HIGH RESOLUTION GHZ AND THZ (FTIR) SPECTROSCOPY AND THEORY OF PARITY VIOLATION AND TUNNELING FOR 1,2-DITHIINE ($C_4H_4S_2$) AS A CANDIDATE FOR MEASURING THE PARITY VIOLATING ENERGY DIFFERENCE BETWEEN ENANTIOMERS OF CHIRAL MOLECULES

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We report high resolution spectroscopic results for 1,2-dithiine-(1,2-dithia-3,5-cyclohexadiene,$C_4H_4S_2$) in the Gigahertz and Terahertz spectroscopic ranges and exploratory theoretical calculations of parity violation and tunneling processes in view of a possible experimental determination of the parity violating energy difference $\Delta_{pv}E$ in this chiral molecule.[a,b] Theory predicts that the parity violating energy difference in the ground state ($\Delta_{pv}E \simeq 11\text{x}10^{-11}(hc)\ \mathrm{cm}^{-1}$)is in principle measurable as it is much larger than the calculated tunneling splitting for the symmetrical potential $\Delta_{\pm}E \simeq 10^{-24}(hc)\ \mathrm{cm}^{-1}$. With a planar transition state for stereomutation at about 2500 cm^{-1}tunneling splittings become appreciable above 2300 cm^{-1}. This makes levels of well defined parity accessible to parity selection by available powerful infrared lasers and thus useful for one of the existing experimental approaches towards molecular parity violation.[c] The new GHz spectra lead to greatly improved ground state rotational parameters for 1,2-dithiine. These are used as starting point for the first successful analyses of high resolution interferometric Fourier Transform Infrared (FTIR, THz) spectra for the fundamentals ν_{17} (1308.873 cm^{-1}or 39.23903 THz), ν_{22} (623.094 cm^{-1}or 18.67989 THz) and ν_3 (1544.900 cm^{-1}or 46.314937 THz) for which highly accurate spectroscopic parameters are reported. The results are discussed in relation to current efforts to measure $\Delta_{pv}E$.[a-d]

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[b] S. Albert, I. Bolotova, Z. Chen, C. Fábri, L. Horný, M. Quack, G. Seyfang and D. Zindel,Proceedings of the 20th Symposium on Atomic, Cluster and Surface Physics (SASP 2016), Innsbruck University Press, 2016, pp. 127-130, ISBN:978-3-903122-04-8. and to be published

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